

Atmospheric Pollution Research

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A two dimensional numerical model of primary pollutant emitted from an urban area source with mesoscale wind, dry deposition and chemical reaction

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ABSTRACT

A two dimensional numerical model has been developed to study the dispersion of a primary pollutant emitted from an urban area source in the presence of mesoscale wind. The model takes into account the transformation and removal mechanisms through chemical reaction, dry deposition and gravitational settling processes. The numerical model is solved using the Crank–Nicolson finite difference scheme under the stability dependent meteorological parameters involved in wind velocities and eddy diffusivity profiles. The urban heat island effect generates its own mesoscale winds and consequently prevents the dispersal of pollutants which will result in an increase in the concentration of pollution in the atmosphere. The analysis shows that the mesoscale wind reduces the concentration of a primary pollutant in the upwind side of centre of heat island and increases the concentration in the downwind side of centre of heat island.

Keywords: Primary pollutant, mesoscale wind, Crank–Nicolson method, dry deposition, gravitational settling



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Article History:

Received: 15 September 2012

Revised: 11 November 2012

Accepted: 12 November 2012

doi: 10.5094/APR.2013.011

1. Introduction

The dispersion of air pollutants from an area source into the atmosphere is governed by the processes of molecular diffusion and convection and depends upon the factors such as wind speed, temperature inversion, and dry deposition. The dispersion of atmospheric contaminants has become a global problem in the recent years due to rapid industrialization and urbanization. The toxic gases and small particles could accumulate in large quantities over urban areas, under certain meteorological conditions. This is one of the serious health hazards in many of the cities in the world. An acute exposure to the elevated levels of particulate air pollution has been associated with the cases of increased cardiopulmonary mortality, hospitalization for respiratory diseases, exacerbation of asthma, decline in lung function, and restricted life activity. Small deficits in lung function, higher risk of chronic respiratory disease and increased mortality have also been associated with chronic exposure to respirable particulate matter (Pope et al., 1995). Epidemiological studies have demonstrated a consistent increased risk for cardiovascular functions in relation to both short- and long-term exposure to the present-day concentrations of ambient particulate matter (Brook et al., 2004). Exposure to the fine airborne particulate matter is associated with cardiovascular functions and mortality in older and cardiac patients (Riediker et al., 2004). Volatile organic compounds (VOCs) are considered a major source of indoor air pollution and have been associated with

various adverse health effects including infection and irritation of respiratory tract, irritation to eyes, allergic skin reaction, bronchitis, and dyspnea (Oke, 1995; Mölders and Olson, 2004; Arif and Shah, 2007). Principal sources of air-pollution are industries, automobiles and household indoor pollutants. The life cycle of pollutants includes emission, dispersion and removal by dry deposition on the surface of the earth. One of the most effective ways to assess the impact of various pollutants on the environment of a particular area is through mathematical modeling. Mathematical models are important tools and can play a crucial role in the methodology developed to predict air quality.

Sometimes the pollutant appears in the form of larger particles on which the effect of gravitational acceleration cannot be neglected (Calder, 1961). In this case the pollutant will come down to the surface by means of gravitational settling velocity W_s . Particles less than 20 μm are treated as gases, and effects due to their fall velocity are generally ignored. Particles greater than 20 μm have appreciable settling velocities. A particular pollutant emitted into the atmosphere may be removed by a number of natural processes. For example, dry deposition fluxes of reactive nitrogen species are not only influenced by micrometeorological and plant-physiological parameters, but also strongly affected by chemical reactions (Kramm and Dlugi, 1994; Kramm et al., 1995).

Tetzlaff et al. (2002) and Zhang et al. (2003) have examined the effect of gravitational settling and ground absorption in the study of air pollution models. The study of chemically reactive heavy admixture and its byproducts has generated considerable attention because of their severe harmful effect on human beings and the environment. A part of an atmospheric contaminant and its byproduct might occur in the form of a particle due to the complexity of the nature of the atmosphere. The particles (or heavy admixture) and their movement by gravitational acceleration have a significant impact on the local ecosystem. Therefore, it is imperative to have a mathematical model to study the concentration of the primary pollutants due to chemical reaction and their removal by means of gravitational settling.

It is well known that large urban areas often generate their own mesoscale winds due to urban heat sources (Dilley and Yen, 1971; Oke, 1995). Consequently, knowledge of the large-scale wind is not sufficient for air pollution forecast in urban areas. The simplest area source model is the box model in which the pollutants are assumed to be completely mixed within a single box, covering the city and extend upward to the mixing height. The application of this single box model, including time dependency, has been discussed by Lettau (1970). Further, this single box model has been extended by Reiquam (1970), which consists of a horizontal array of boxes in the x - y -plane along the ground surface. Ragland (1973) has developed a multiple box model for the dispersion of air pollutants from an area source. Sheih (1977) has developed a generalized urban air pollution model and applied to the study of SO_2 distribution. Gryng et al. (1983) have studied the dispersion from the continuous ground level source using the K -theory model. Nokes et al. (1984) have developed a model to study turbulent dispersion of a steady two-dimensional horizontal source. Most of the above models are analytical in nature with simple form of wind velocity and eddy diffusivity under restrictive assumptions without mesoscale wind.

Davidson (1967) and Chandler (1968) have commented that near the center of a heat island, the vertical mixing would be enhanced by mesoscale wind. There are numerous models (Dilley and Yen, 1971) dealing with the dispersion of pollutants emitted from point, line and area sources. Rudraiah et al. (1997) have studied the atmospheric diffusion model of secondary pollutants with settling. Khan (2000) and Venkatachalappa et al. (2003) have presented a time dependent mathematical model of an air pollutant with instantaneous and delayed removal. Lakshminarayanachari et al. (2011) have studied the mathematical model with chemically reactive pollutants without considering mesoscale wind. In these

models eddy-diffusivity and velocity profiles are all considered constant and they do not deal with the effect of mesoscale wind. Pandurangappa et al. (2011) have presented a two dimensional numerical model with mesoscale wind. However, they have not considered the effect of the gravitational settling velocity.

In this paper we present a numerical model for a primary pollutant in the atmosphere taking into account, the large scale and mesoscale wind velocities and eddy diffusivity profiles. We study the effect of removal mechanisms such as dry deposition and gravitational settling velocity on the primary pollutants along with the chemical reactions involved.

2. Model Development

The physical problem consists of an area source, which is spread over the surface of a city with finite downwind distance and infinite cross wind dimensions. We assume that the pollutants are emitted at a constant rate from the area source and spread within the mixing layer adjacent to the earth's surface where mixing takes place as a result of turbulence and convective motion of wind. This mixing layer extends upwards from the surface to a height where all turbulent flux-divergences resulting from surface action have virtually fallen to zero. The pollutants are transported horizontally by a large scale wind which is a function of vertical height (z) and horizontally as well as vertically by the local wind caused by the urban heat source, called mesoscale wind.

We have considered the centre of the heat island at a distance $x=l/2$ i.e. at the centre of the city. We have considered the source region within the urban area which extends to a distance l , where l is the city length and x is the distance in the horizontal downwind direction $0 \leq x \leq l$. In this model, we have taken $l=6$ km. Assuming the homogeneity of urban terrain, the mean concentration of pollutant is considered to be a constant along the crosswind direction i.e., pollutants concentration does not vary in cross wind direction. Therefore, there is no y -dependence. Also, the lateral flux of the pollutants is small and it traverses the centre line of uniform area source. The meteorological parameters influencing eddy diffusivity and velocity profile are dependent on the intensity of turbulence, which is influenced by atmospheric stability. The physical description of the model is shown schematically in Figure 1. We intend to compute the concentration distribution in the urban area. We assume that the pollutants undergo the removal mechanisms, i.e., dry deposition, wet deposition and gravitational settling.

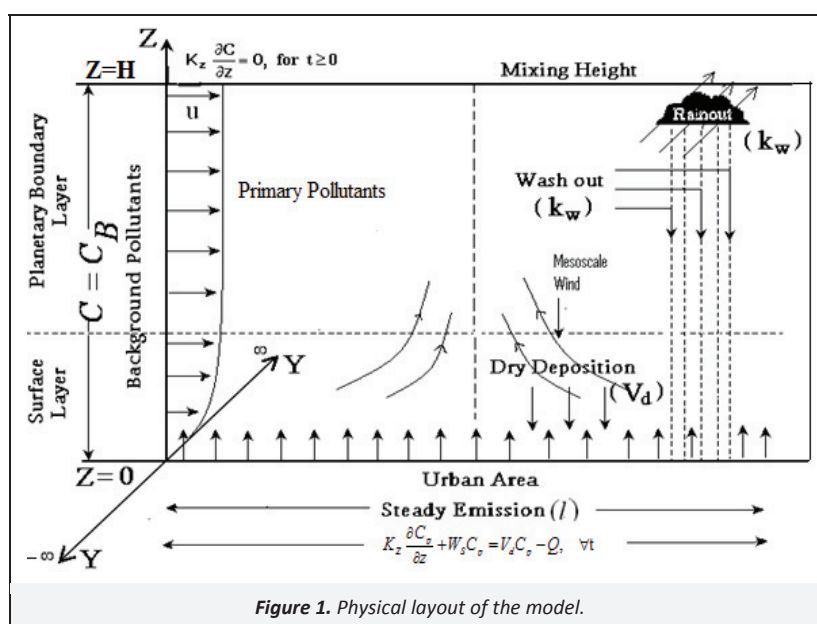


Figure 1. Physical layout of the model.

2.1. Primary pollutant

The basic governing equation of the primary pollutant (Pasquill and Smith, 1983) can be written as:

$$\frac{\partial C_p}{\partial t} + U(x, z) \frac{\partial C_p}{\partial x} + W(z) \frac{\partial C_p}{\partial z} = \frac{\partial}{\partial z} \left(K_z(z) \frac{\partial C_p}{\partial z} \right) - (k + k_{wp}) C_p \quad (1)$$

where $C_p = C_p(x, z, t)$ is the ambient mean concentration of the pollutant species, U is the mean wind speed in x -direction, W is the mean wind speed in z -direction, K_z is the turbulent eddy diffusivity in z -direction and k is the first order chemical reaction rate coefficient of primary pollutant C_p , k_{wp} is the first order rainout/ washout coefficient of primary pollutant C_p . Equation (1) is derived under the following assumptions:

- The lateral flux of the pollutants along crosswind direction is assumed to be small i.e., $V(\partial C_p / \partial y)$ and $\partial / \partial y [K_y(\partial C_p / \partial y)] \rightarrow 0$ where V is the velocity in the y -direction and K_y is the eddy-diffusivity coefficient in the y direction.
- The horizontal advection is greater than the horizontal diffusion for not too small values of wind velocity, i.e., meteorological conditions being far from stagnation. The horizontal advection by the wind dominates over the horizontal diffusion, i.e., $U(\partial C_p / \partial x) \gg \partial / \partial x [K_x(\partial C_p / \partial x)]$ where U and K_x are the horizontal wind velocity and the horizontal eddy diffusivity along the x -direction respectively.
- The vertical diffusion is greater than the vertical advection since the vertical advection is usually negligible compared to the diffusion due to the small vertical component of the wind velocity.

We assume that the region of interest is free from pollution at the beginning of the emission. Thus, the initial condition is:

$$C_p = 0 \quad \text{at } t = 0, \quad 0 \leq x \leq l \quad \text{and} \quad 0 \leq z \leq H \quad (2)$$

where l is the city length in the horizontal direction and H is the mixing height. We assume that there is no background concentration of pollution entering at $x=0$ into the domain of interest. Thus,

$$C_p = 0 \quad \text{at } x = 0, \quad 0 \leq z \leq H \quad \text{and} \quad \forall t > 0 \quad (3)$$

We assume that the chemically reactive air pollutants are being emitted at a steady rate from the ground level. They are removed from the atmosphere by ground adsorption. Hence the corresponding boundary condition takes the form:

$$K_z \frac{\partial C_p}{\partial z} + W_s C_p = V_{dp} C_p - Q \quad (4)$$

at $z = 0, \quad 0 < x \leq l \quad \text{and} \quad \forall t > 0$

where W_s is the gravitational settling velocity of the primary pollutant, $C_p Q$ is the emission rate of primary pollutant species and V_{dp} is the dry deposition velocity. The pollutants are confined within the mixing height and there is no leakage across the top boundary of the mixing layer. Thus,

$$K_z \frac{\partial C_p}{\partial z} = 0 \quad (5)$$

at $z = H, \quad x > 0, \quad 0 < x \leq l \quad \text{and} \quad \forall t > 0$

The term kC_p in Equation (1) represents the conversion of gaseous pollutants to particulate material as long as the process can be represented approximately by the first-order chemical

reaction. Bimolecular, three-body, photolysis and thermal decomposition are some the chemical reactions which take place in the atmosphere to form secondary pollutants and secondary aerosols. We assume that the gaseous species is converted into a particulate matter. Sulfates, nitrates, ammonium salts are examples of gas-to-particle conversion.

3. Meteorological Parameters

The treatment of Equation (1) mainly depends on the proper estimation of the diffusivity coefficient and the velocity profile of the wind near the ground/or the lower layers of the atmosphere. The meteorological parameters influencing eddy diffusivity and velocity profile are dependent on the intensity of turbulence, which is influenced by atmospheric stability. Stability near the ground is dependent primarily upon the net heat flux. In terms of the boundary layer notation, the atmospheric stability is characterized by the parameter L (Monin and Obukhov, 1954), which is also a function of net heat flux among several other meteorological parameters. It is defined by:

$$L = - \frac{u_*^3 \rho C_p T}{\kappa g H_f} \quad (6)$$

where u_* is the friction velocity, H_f the net heat flux, ρ the ambient air density, C_p the specific heat at constant pressure, T the ambient temperature near the surface, g the gravitational acceleration and κ the Karman constant ≈ 0.4 . $H_f < 0$ and consequently $L > 0$ represents stable atmosphere, $H_f > 0$ and $L < 0$ represent unstable atmosphere and $H_f = 0$ and $L \rightarrow \infty$ represent neutral condition of the atmosphere.

The friction velocity u_* is defined in terms of geostrophic drag coefficient c_a and geostrophic wind u_g such that

$$u_* = c_g u_g \quad (7)$$

where c_g is a function of the surface Rossby number, $Ro = u_g / f z_0$ where f is the Coriolis parameter due to the earth's rotation and z_0 is the surface roughness length. Lettau (1959) gave the value of c_{gn} the drag coefficient for a neutral atmosphere in the form of:

$$c_{gn} = \frac{0.16}{\log_{10}(Ro) - 1.8} \quad (8)$$

The effect of thermal stratification on the drag coefficient (Lettau, 1959) can be accounted through the relations:

$$c_{gus} = 1.2 c_{gn} \quad (9)$$

for unstable flow,

$$c_{gs} = 0.8 c_{gn} \quad (10)$$

for slightly stable flow and

$$c_{gs} = 0.6 c_{gn} \quad (11)$$

for stable flow.

To evaluate the drag coefficient, the surface roughness length z_0 may be computed according to the relationship developed by Lettau (1970) i.e., $z_0 = (\bar{H} a) / (2 \bar{A})$, where \bar{H} is the effective height of roughness elements, a is the frontal area seen by the wind and \bar{A} is the lot area (i.e. the total area of the region divided by the number of elements).

Finally, in order to connect the stability length L to the Pasquill stability categories, it is necessary to quantify the net radiation index. Ragland (1973) used the following values of H_f (Table 1) for urban area.

Table 1. Net heat flux H_f (langley min^{-1})

| | | | | | | | |
|---------------------|---|------|------|------|-----|-------|-------|
| Net radiating index | 4 | 3.0 | 2.0 | 1.0 | 0.0 | -1.0 | -2.0 |
| Net heat flux H_f | 0 | 0.18 | 0.12 | 0.06 | 0.0 | -0.03 | -0.06 |

3.1. Eddy diffusivity profiles

Following the gradient transfer hypothesis and dimensional analysis, the eddy viscosity K_M is defined as:

$$K_M = \frac{u_*^2}{\partial U / \partial z} \quad (12)$$

Using Monin and Obukhov's (1954) similarity theory, the velocity gradient may be written as:

$$\frac{\partial U}{\partial z} = \frac{u_* \phi_M}{\kappa z} \quad (13)$$

Substituting Equation (13) in Equation (12), we have:

$$K_M = \frac{\kappa u_* z}{\phi_M} \quad (14)$$

the function ϕ_M depends on, z/L where L is Monin–Obukhov stability length parameter. It is assumed that the surface layer terminates at $z=0.1 \kappa (u_*/f)$ for neutral stability. For stable conditions, surface layer extends to $z=6L$.

For neutral stability with $z < 0.1 \kappa (u_*/f)$ (within surface layer),

$$\phi_M = 1 \text{ and } K_M = \kappa u_* z \quad (15)$$

for stable flow with $0 < z/L < 1$,

$$\phi_M = 1 + \frac{\alpha}{L} z \quad (16)$$

and

$$K_M = \frac{\kappa u_* z}{1 + \frac{\alpha}{L} z} \quad (17)$$

for stable flow with $1 < z/L < 6$,

$$\phi_M = 1 + \alpha \text{ and } K_M = \frac{\kappa u_* z}{1 + \alpha} \quad (18)$$

Webb (1970) has shown that $\alpha=5.2$. In the planetary boundary layer, where z/L is greater than the limits considered above and $z > 0.1 \kappa (u_*/f)$, we have, the following expressions for K_M :

for neutral stability with $z > 0.1 \kappa (u_*/f)$,

$$K_M = 0.1 \kappa^2 \frac{u_*^2}{f} \quad (19)$$

for stable flow with $z > 6L$, up to H , the mixing height,

$$K_M = \frac{6 \kappa u_* L}{1 + \alpha} \quad (20)$$

Equations (14) to (20) give the eddy viscosity for the conditions needed for the model. However, the model deals with the transport of mass rather than the transport of momentum, as implied by the use of viscosity. Since both the mass and the momentum are transported by turbulent eddies, it is physically reasonable to assume that the turbulent viscosity coefficient K_M is numerically equivalent to the eddy diffusivity coefficient, K_z . Also, there is some experimental evidence that the ratio K_z/K_M remains constant and equal to unity, at least in the surface layer as shown by Webb (1970). The common characteristic of K_z is that it has a linear variation near the ground, a constant value at mid mixing depth and a decreasing trend as the top of the mixing layer is approached. Shir (1973) gave such an expression, based on theoretical analysis of neutral boundary layer, in the form,

$$K_z = 0.4 u_* z e^{-4z/H} \quad (21)$$

where H is the mixing height.

For stable condition, Ku et al. (1987) used the following form of eddy-diffusivity,

$$K_z = \frac{\kappa u_* z}{0.74 + 4.7z/L} \exp(-b\eta), \quad b = 0.91, \quad (22)$$

$$\eta = z/(L\sqrt{\mu}), \quad \mu = u_*/|fL|$$

The above form of K_z was derived from a higher order turbulence closure model which was tested with stable boundary layer data of Kansas and Minnesota experiments.

Eddy-diffusivity profiles given by Equations (21) and (22) have been used in this model developed for neutral and stable atmospheric conditions.

3.2. Mesoscale wind velocity profiles

It is known that in an urban area the heat generation causes the vertical flow of air with maximum velocity (rising of air) at the centre of the city (Oke, 1995). Hence the city can be called a heat island. This rising air forms a circulation and this circulation is completed at larger heights. This is called a mesoscale circulation. To incorporate a more realistic form of velocity profile in the models, we integrate equation $(\partial U / \partial z) = (u_* \phi_M / \kappa z)$ from z_0 to $z+Z_0$ for stable and neutral conditions which depend on Coriolis force, surface friction, geostrophic wind, stability characteristic parameter L and vertical height z . The velocity profiles of the above models are not sufficient to predict the distribution of concentration over the urban areas. Dilley and Yen (1971) have considered the mesoscale wind velocity profiles for simple power law profile of the large scale wind. Therefore, to take into account the mesoscale wind over the urban areas, for realistic form of velocity profiles, it is necessary to modify the wind velocity profiles of Ragland (1973) as per Dilley and Yen (1971). So, we obtain the following expressions for large and mesoscale wind velocities.

In the case of neutral stability with $z < 0.1 \kappa (u_*/f)$, we get,

$$U = \frac{u_*}{\kappa} \ln \left(\frac{z + Z_0}{z_0} \right) \quad (23)$$

It is assumed that the horizontal mesoscale wind varies in the same vertical manner as u . The vertical mesoscale wind velocity W_e can then be found by integrating the continuity equation and we obtain:

$$U_e = -a(x - x_0) \ln \left(\frac{z + Z_0}{z_0} \right) \quad (24)$$

where U_e is the mesoscale wind velocity along the horizontal direction and a is proportionality constant. Thus we have,

$$U(x, z) = u + u_e = \left(\frac{u_*}{\kappa} - a(x - x_o) \right) \ln \left(\frac{z + z_0}{z_0} \right) \quad (25)$$

$$W(z) = W_e = a \left[z \ln \left(\frac{z + z_0}{z_0} \right) - z + z_0 \ln(z + z_0) \right] \quad (26)$$

in the case of stable flow with $0 < z/L < 1$, we get,

$$U = \frac{u_*}{\kappa} \left[\ln \left(\frac{z + z_0}{z_0} \right) + \frac{\alpha}{L} z \right] \quad (27)$$

$$U_e = -a(x - x_o) \left[\ln \left(\frac{z + z_0}{z_0} \right) + \frac{\alpha}{L} z \right] \quad (28)$$

$$U(x, z) = u + u_e = \left(\frac{u_*}{\kappa} - a(x - x_o) \right) \left[\ln \left(\frac{z + z_0}{z_0} \right) + \frac{\alpha}{L} z \right] \quad (29)$$

$$W(z) = W_e = a \left[z \ln \left(\frac{z + z_0}{z_0} \right) - z + z_0 \ln(z + z_0) + \frac{\alpha}{2L} z^2 \right] \quad (30)$$

in the case of stable flow with $1 < z/L < 6$, we get,

$$U = \frac{u_*}{\kappa} \left[\ln \left(\frac{z + z_0}{z_0} \right) + 5.2 \right] \quad (31)$$

$$U_e = -a(x - x_o) \left[\ln \left(\frac{z + z_0}{z_0} \right) + 5.2 \right] \quad (32)$$

$$U(x, z) = u + u_e = \left(\frac{u_*}{\kappa} - a(x - x_o) \right) \left[\ln \left(\frac{z + z_0}{z_0} \right) + 5.2 \right] \quad (33)$$

$$W(z) = W_e = a \left[z \ln \left(\frac{z + z_0}{z_0} \right) + z_0 \ln(z + z_0) + 4.2z \right] \quad (34)$$

In the planetary boundary layer, above the surface layer, power law scheme has been employed.

$$U = (u_g - u_{sl}) \left(\frac{z - z_{sl}}{H - z_{sl}} \right)^p + u_{sl} \quad (35)$$

$$U_e = -a(x - x_o) \left[\left(\frac{z - z_{sl}}{H - z_{sl}} \right)^p + u_{sl} \right] \quad (36)$$

$$U(x, z) = u + u_e = [(u_g - u_{sl}) - a(x - x_o)] \left[\left(\frac{z - z_{sl}}{H - z_{sl}} \right)^p + (1 - a(x - x_o))u_{sl} \right] \quad (37)$$

$$W(z) = W_e = a \left[\frac{(z - z_{sl})}{p + 1} \left(\frac{z - z_{sl}}{H - z_{sl}} \right)^p + zu_{sl} \right] \quad (38)$$

where, u_g is the geostrophic wind, u_{sl} the wind at z_{sl} . z_{sl} the top of the surface layer, H the mixing height and p is an exponent which depends upon the atmospheric stability. Jones et al. (1971) have suggested the values for the exponent p , obtained from the measurements made from the urban wind profiles, as follows:

$$p = \begin{cases} 0.20 & \text{for neutral condition} \\ 0.35 & \text{for slightly stable flow} \\ 0.50 & \text{for stable flow} \end{cases}$$

Wind velocity profiles given by Equations (29), (30), (33), (34), (37) and (38) (Dilley and Yen, 1971) are used in this model.

4. Numerical Method

It is to be noted that it is difficult to obtain the analytical solution for Equations (1) and (6) because of the complicated form

of wind speed and eddy diffusivity profiles considered in this model. Hence, we have used the numerical method based on the Crank–Nicolson finite difference scheme to obtain the solution. The dependent variable C_p is a function of the independent variables x , z and t , i.e., $C_p = C_p(x, z, t)$. First, the continuum region of interest is overlaid with or subdivided into a set of equal rectangles of sides Δx and Δz , by equally spaced gridlines, parallel to z axis, defined by $x_i = (i-1)\Delta x$, $i=1,2,3,\dots$ and equally spaced grid lines parallel to x axis, defined by $z_j = (j-1)\Delta z$, $j=1,2,3,\dots$ respectively. Time is indexed such that $t_n = n\Delta t$, $n=1,2,3,\dots$, where Δt is the time step. At the intersection of gridlines, i.e. grid points, the finite difference solution of the variable C_p is defined. The dependent variable $C_p(x, z, t)$ is denoted by $C_{pij}^n = C_p(x_i, z_j, t_n)$, where (x_i, z_j) and t_n indicate the (x, z) value at a node point (i, j) and t value at time level n respectively.

We employ the implicit Crank–Nicolson scheme to discretize the Equation (1). The derivatives are replaced by the arithmetic average of their finite difference approximations at the n^{th} and $(n+1)^{th}$ time steps. Then Equation (1) at the grid points (i, j) and time step $n+1/2$ can be written as:

$$\begin{aligned} & \frac{\partial C_p}{\partial t} \Big|_{ij}^{n+1/2} + \frac{1}{2} \left[U(z) \frac{\partial C_p}{\partial x} \Big|_{ij}^n + U(z) \frac{\partial C_p}{\partial x} \Big|_{ij}^{n+1} \right] \\ & + \frac{1}{2} \left[W(z) \frac{\partial C_p}{\partial z} \Big|_{ij}^n + W(z) \frac{\partial C_p}{\partial z} \Big|_{ij}^{n+1} \right] = \\ & \frac{1}{2} \left[\frac{\partial}{\partial z} \left(K_z(z) \frac{\partial C_p}{\partial z} \right) \Big|_{ij}^n + \frac{\partial}{\partial z} \left(K_z(z) \frac{\partial C_p}{\partial z} \right) \Big|_{ij}^{n+1} \right] \\ & - \frac{1}{2} (k + k_{wp}) (C_{pij}^n + C_{pij}^{n+1}) \end{aligned} \quad (39)$$

for $i = 1, 2, \dots, j = 1, 2, \dots$

This analog is actually the same as the first-order correct analog used for the forward difference equation, but is now the second-order-correct, since it is used to approximate the derivative at the point $(x_i, z_j, t_{n+1/2})$.

We use the backward differences for advective term in the primary pollutant equation:

$$\frac{\partial C_p}{\partial t} \Big|_{ij}^{n+1/2} = \frac{C_{pij}^{n+1} - C_{pij}^n}{\Delta t}$$

The simplest way to model the transport properties is to use upwind differencing where backward differences are used when the velocities are positive and forward differences are used when the velocities are negative.

$$U(x, z) \frac{\partial C_p}{\partial x} \Big|_{ij}^n = \begin{cases} U_{ij} \left[\frac{C_{pij}^n - C_{pi-1j}^n}{\Delta x} \right] & \text{for } U_{ij} > 0 \\ U_{ij} \left[\frac{C_{pi+1j}^n - C_{pij}^n}{\Delta x} \right] & \text{for } U_{ij} < 0 \end{cases} \quad (40)$$

It is noted that in the present problem the velocity is always positive and hence we always use:

$$U(x, z) \frac{\partial C_p}{\partial x} \Big|_{ij}^n = U_{ij} \left[\frac{C_{pij}^n - C_{pi-1j}^n}{\Delta x} \right] \quad (41)$$

$$U(x, z) \frac{\partial C_p}{\partial x} \Big|_{ij}^{n+1/2} = U_{ij} \left[\frac{C_{pij}^{n+1} - C_{pi-1j}^{n+1}}{\Delta x} \right] \quad (42)$$

$$W(z) \frac{\partial C_p}{\partial z} \Big|_{ij}^n = W_j \left[\frac{C_{pij}^n - C_{pij-1}^n}{\Delta z} \right] \quad (43)$$

$$W(z) \frac{\partial C_p}{\partial z} \Big|_{ij}^{n+1} = W_j \left[\frac{C_{pij}^{n+1} - C_{pij-1}^{n+1}}{\Delta z} \right] \quad (44)$$

Also, for the diffusion term, we use the second order central difference scheme,

$$\frac{\partial}{\partial z} \left(K_z(z) \frac{\partial C_p}{\partial z} \right) \Big|_{ij}^n = \frac{K_z(z) \frac{\partial C_p}{\partial z} \Big|_{ij+1/2}^n - K_z(z) \frac{\partial C_p}{\partial z} \Big|_{ij-1/2}^n}{\Delta z} =$$

$$\frac{1}{\Delta z} \left(\frac{K_{j+1} + K_j}{2} \right) \left(\frac{C_{pij+1}^n - C_{pij}^n}{\Delta z} \right) - \frac{1}{\Delta z} \left(\frac{K_j + K_{j-1}}{2} \right) \left(\frac{C_{pij}^n - C_{pij-1}^n}{\Delta z} \right)$$

hence,

$$\frac{\partial}{\partial z} \left(K_z(z) \frac{\partial C_p}{\partial z} \right) \Big|_{ij}^n = \frac{1}{2(\Delta z)^2} \left[(K_{j+1} + K_j)(C_{pij+1}^n - C_{pij}^n) - (K_j + K_{j-1})(C_{pij}^n - C_{pij-1}^n) \right] \quad (45)$$

similarly,

$$\frac{\partial}{\partial z} \left(K_z(z) \frac{\partial C_p}{\partial z} \right) \Big|_{ij}^{n+1} = \frac{1}{2(\Delta z)^2} \left[(K_{j+1} + K_j)(C_{pij+1}^{n+1} - C_{pij}^{n+1}) - (K_j + K_{j-1})(C_{pij}^{n+1} - C_{pij-1}^{n+1}) \right] \quad (46)$$

Substituting Equations (43) to (45) in Equation (46) and rearranging the terms we get the finite difference equations for the primary pollutant C_p in the form of:

$$A_j C_{pi-1j}^{n+1} + B_j C_{pij-1}^{n+1} + D_j C_{pij}^{n+1} + E_j C_{pij+1}^{n+1} = F_j C_{pi-1j}^n + G_j C_{pij-1}^n + M_j C_{pij}^n + N_j C_{pij+1}^n \quad (47)$$

for each $i=2,3,4,...imaxl...imaxX_0$, for each $j=2,3,4,...jmax-1$ and $n=0,1,2,3,...$

Where,

$$A_j = -U_j \frac{\Delta t}{2\Delta x} \quad F_j = U_j \frac{\Delta t}{2\Delta x}$$

$$B_j = - \left[\frac{\Delta t}{4(\Delta z)^2} (K_j + K_{j-1}) + W_j \frac{\Delta t}{2\Delta z} \right]$$

$$G_j = \left[\frac{\Delta t}{4(\Delta z)^2} (K_j + K_{j-1}) + W_j \frac{\Delta t}{2\Delta z} \right]$$

$$E_j = - \frac{\Delta t}{4(\Delta z)^2} (K_j + K_{j+1})$$

$$N_j = \frac{\Delta t}{4(\Delta z)^2} (K_j + K_{j+1})$$

$$D_j = 1 + U_j \frac{\Delta t}{2\Delta x} + W_j \frac{\Delta t}{2\Delta z} + \frac{\Delta t}{4(\Delta z)^2} (K_{j+1} + 2K_j + K_{j-1}) + \frac{\Delta t}{2} (k + k_{wp})$$

$$M_j = 1 - U_j \frac{\Delta t}{2\Delta x} - W_j \frac{\Delta t}{2\Delta z} - \frac{\Delta t}{4(\Delta z)^2} (K_{j+1} + 2K_j + K_{j-1}) - \frac{\Delta t}{2} (k + k_{wp})$$

$imaxl$ and $imaxX_0$ are the i values at $x=l$ and X_0 respectively and $jmax$ is the value of j at $z=H$.

Equation (47) is true for interior grid points. At the boundary, grid points we have to use the boundary conditions (2) to (5).

The initial condition (2) is,

$$C_{pij}^0 = 0 \text{ for } j = 1, 2, \dots, jmax, \quad i = 1, 2, \dots, imaxl \dots imaxX_0$$

the condition (3) becomes

$$C_{pij}^{n+1} = 0 \text{ for } i = 1 \text{ and } j = 1, 2, \dots, jmax, \quad n = 0, 1, 2, \dots \quad (48)$$

the boundary condition (4) can be written as:

$$\left(1 + [V_d + W_s] \frac{\Delta z}{K_j} \right) C_{pij}^{n+1} - C_{pij+1}^{n+1} = - \frac{Q\Delta z}{K_j} \quad (49)$$

for $j=1, i=2,3,4,...imaxl$ and $n=0,1,2,3,...$

The boundary condition (5) can be written as:

$$C_{pijmax-1}^{n+1} - C_{pijmax}^{n+1} = 0 \text{ for } j = jmax, \quad i = 2, 3, 4, \dots, imaxl \dots imaxX_0 \quad (50)$$

The above system of Equations (47) to (50) has a tridiagonal structure and is solved by Thomas Algorithm (Akai, 1994). The ambient air concentration of the primary pollutants (gaseous) is obtained for stable and neutral atmospheric conditions.

5. Results and Discussion

The results of the above model are presented graphically from Figures 2 to 7 to analyze the dispersion of air pollutants in the urban area downwind and vertical direction for the stable and the neutral conditions of atmosphere. Figure 8 represents the concentration contours of the primary pollutants for both the stable and the neutral cases.

In Figure 2, the effect of mesoscale wind on the concentrations of the primary pollutant with the chemical reaction rate coefficient with respect to distance for the stable and the neutral atmospheric conditions is analyzed. The concentration of the primary pollutant decreases rapidly as the value of the chemical reaction rate increases. The concentration of the pollutant is less in upwind side of the centre of heat island and is higher in the downwind side of the centre of heat island in the presence of mesoscale wind ($\alpha=0.00004$) as compared to that of one without mesoscale wind ($\alpha=0$). This behavior is because, the horizontal component of mesoscale wind is along the large scale wind on the left and against on the right. Thus in the presence of mesoscale wind, the advection is more on the left and less on the right. Therefore, the concentration of the primary pollutant is less on the left and more on the right in the presence of mesoscale wind. In general, the concentration of the primary pollutant increases in the downwind direction. Comparing Figures 2a and 2b, we find that the concentrations of the pollutant at a given distance is much less in the neutral atmospheric condition than in the stable atmospheric case. The maximum concentration of pollutant is around $200 \mu\text{g m}^{-3}$ in the stable case and is near $55 \mu\text{g m}^{-3}$ in the neutral atmosphere at $x=6000$ m.

In Figure 3, the effect of mesoscale wind on the concentration of the primary pollutant with the chemical reaction rate coefficient with respect to height for the stable and the neutral atmospheric conditions with and without mesoscale wind is analyzed. The concentration of the pollutant decreases as the chemical reaction rate increases. The magnitude of concentration of the pollutant is higher in the stable case and lower in the neutral case. This behavior is because the neutral case enhances vertical diffusion at the greater heights and thus the concentration becomes less. The concentration of the pollutant decreases as height increases. In the stable case, the concentration is zero around 25 m height and in neutral case the concentration reaches zero at 110 m height from the ground level.

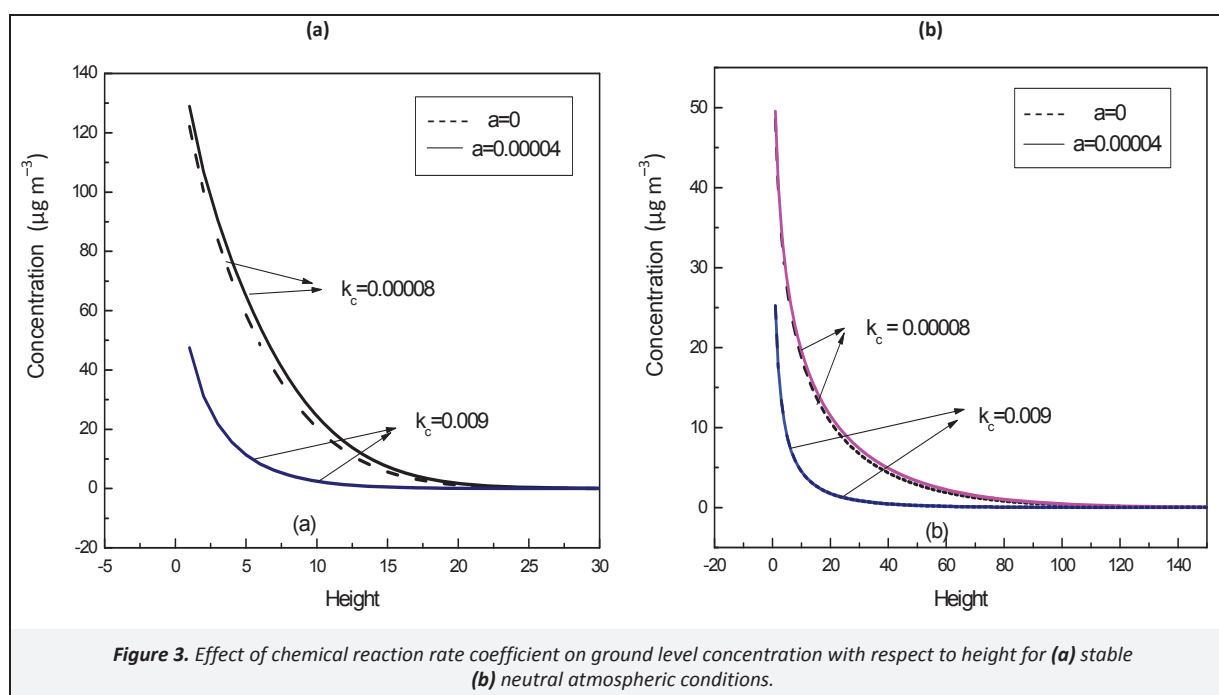
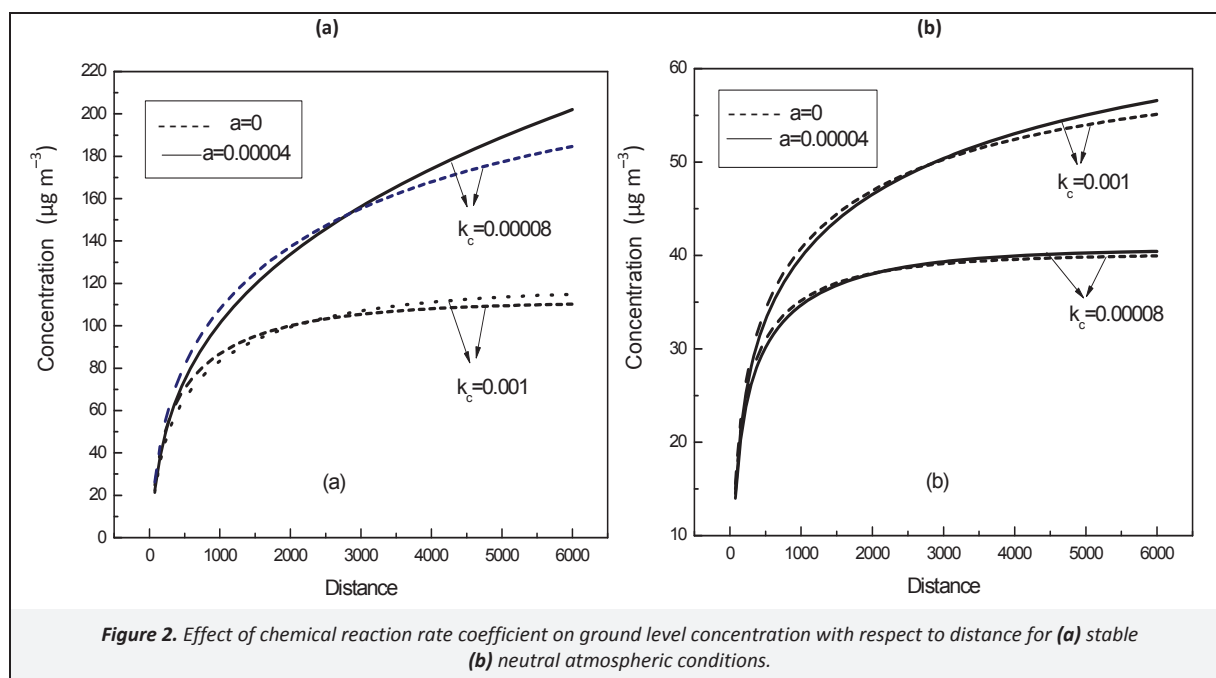
In Figure 4, the effect of mesoscale wind on the concentration of the primary pollutant for different values of the dry deposition velocity with respect to the distance for the stable and the neutral

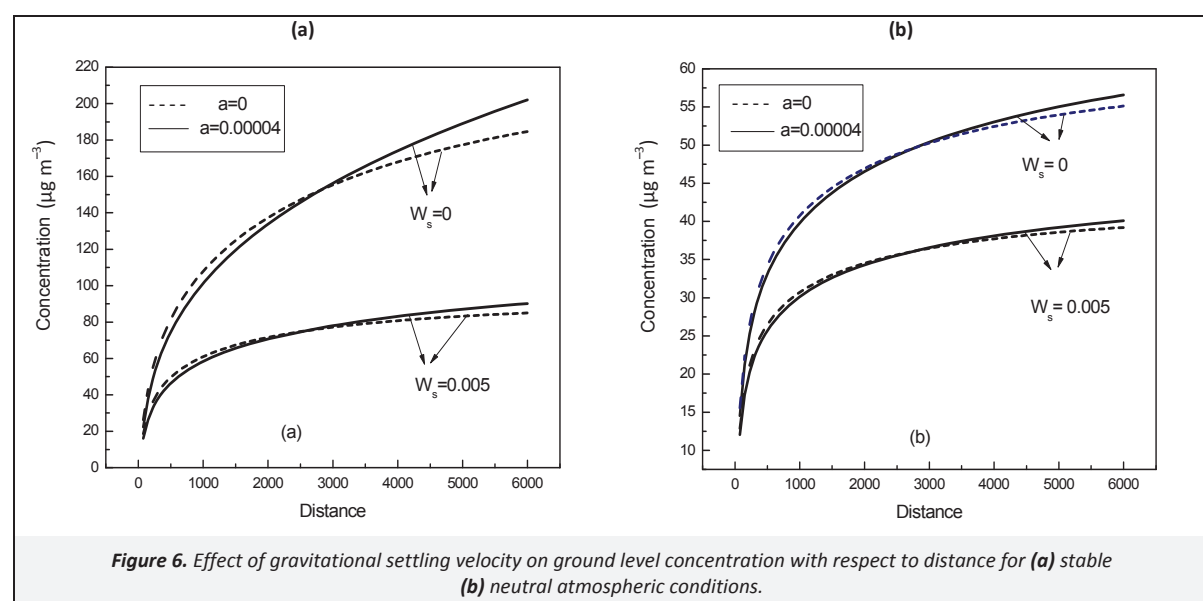
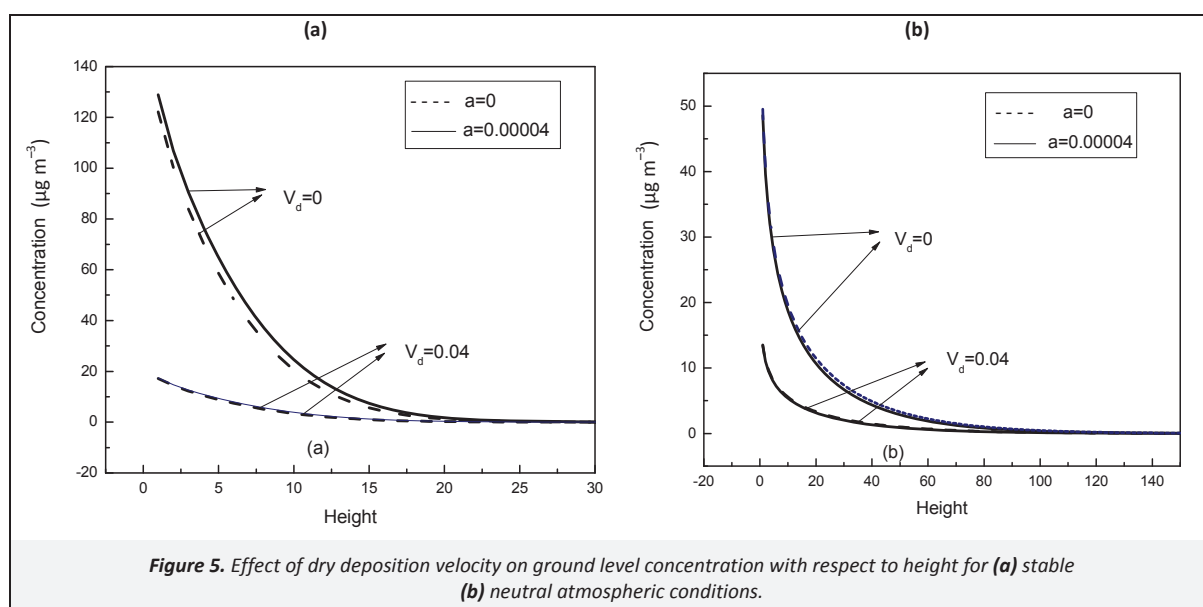
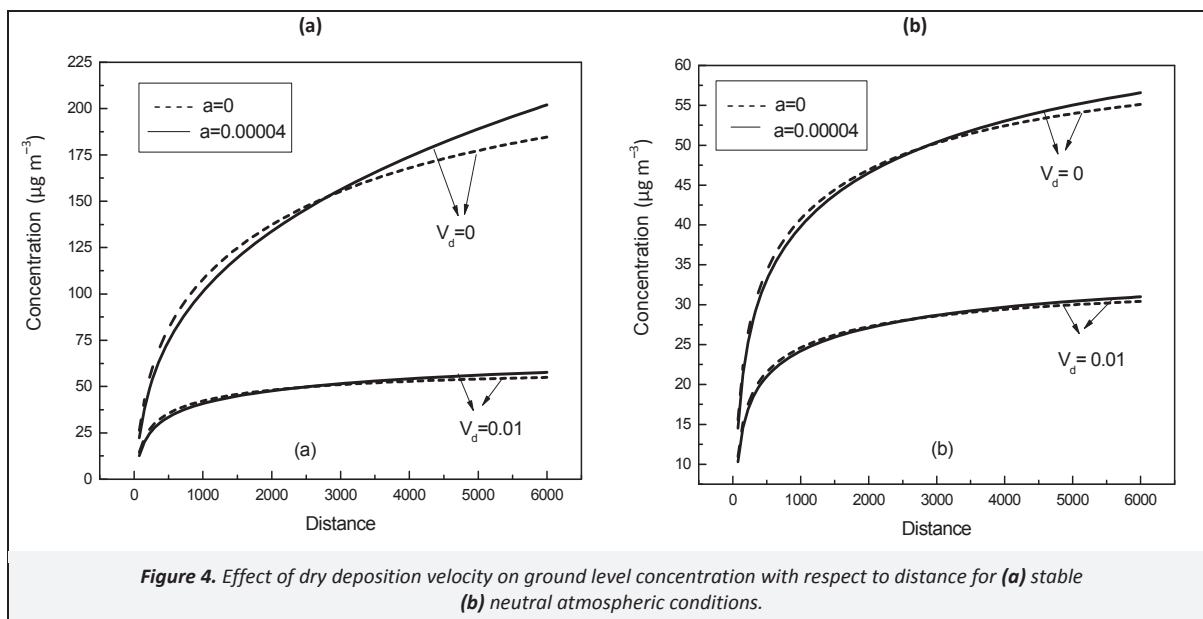
atmospheric conditions is studied. As the dry deposition velocity increases, the concentration of the pollutant decreases. The concentration decreases rapidly in the stable case and decreases slowly in the neutral case because the pollutant's concentration is high in the stable case as compared to one in the neutral case.

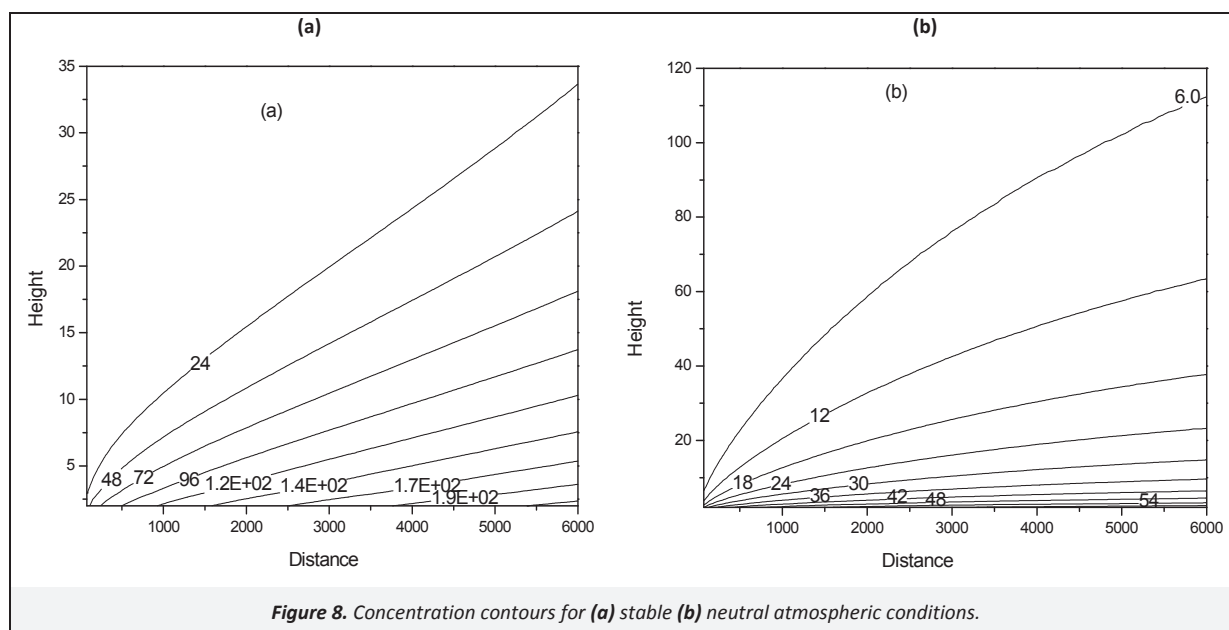
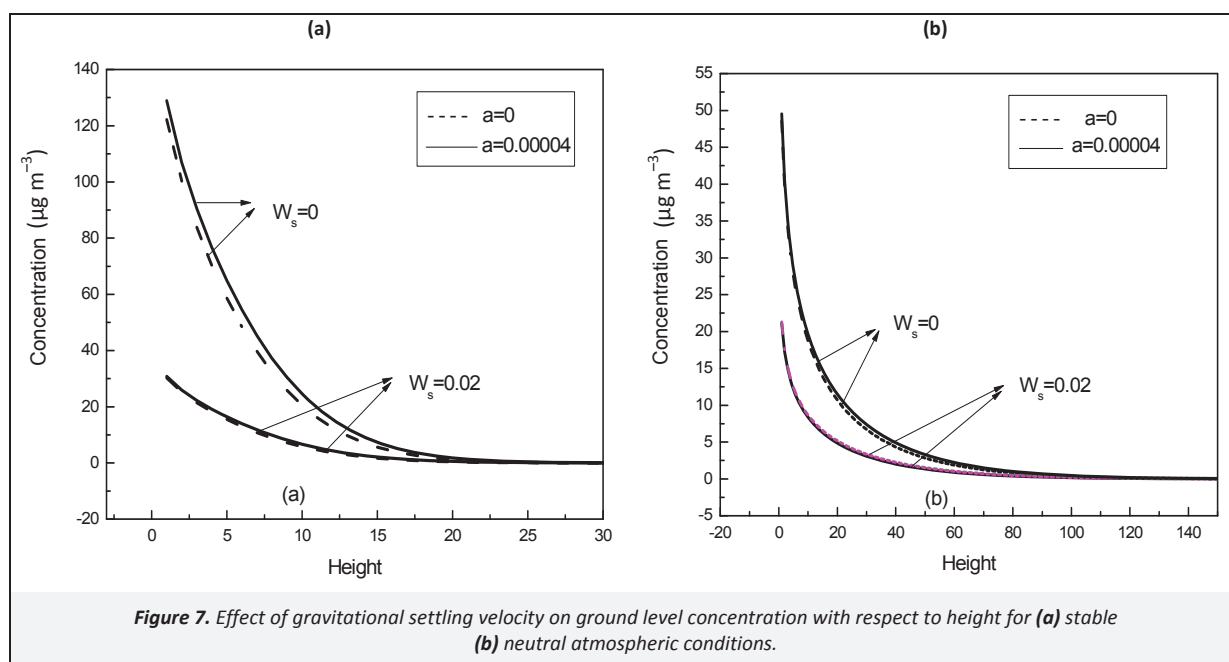
In Figure 5, the effect of mesoscale wind on the concentration of the primary pollutant for different values of the dry deposition velocity with respect to the height for the stable and the neutral atmospheric conditions is studied. As the dry deposition velocity increases, the concentration of the primary pollutant decreases. The magnitude of the pollutant is higher in the stable case and lower in the neutral case. This behavior is because the neutral case enhances the vertical diffusion at the greater heights and thus the

concentration is lower. In the stable case the magnitude of concentration reaches zero around 25 m height and in the neutral case the concentration is zero at 110 m height from the ground level.

In Figure 6, the effect of the gravitational settling velocity with respect to distance in the presence and in the absence of mesoscale wind for the stable and the neutral case is studied. We find that as the gravitational settling velocity increases, the concentration of pollutant decreases. It decreases rapidly in the stable case as compared to the neutral case. We observe that the concentration of the pollutant at a given distance is lower in the neutral case than the one compared to in the stable case.







In Figure 7, the effect of the gravitational settling velocity with respect to the height in the presence and in the absence of mesoscale wind for the stable and the neutral case is studied. Similar effect is observed as in the case of Figure 6. At the ground level, the concentration is higher in the stable case as compared to the neutral atmospheric condition. As the height increases the concentration decreases. It reaches zero at 22 m height in the stable case and the concentration is zero at 110 m height in the neutral atmospheric condition from the ground level.

In Figure 8, the concentration contours of the primary pollutants are plotted for both the stable and the neutral cases. As the distance increases the concentration of primary pollutants also increases. Also, as height increases the concentration of primary pollutants decreases. It is observed that the concentration of primary pollutant is higher at ground level ($z=2$ m) and at the end of the city region ($x=6000$ m). The magnitude of pollutant's concentration is higher in the stable case and is lower in neutral case. This effect is because the neutral case enhances vertical diffusion at the greater heights and thus the concentration is lower.

6. Conclusion

The urban heat island effect generates its own mesoscale winds and consequently prevents the dispersal of the pollutants which will result in an increase in the concentration of the pollution in the atmosphere. The urban heat island adds to the development of haze of contaminated pollutants and also helps these pollutants to circulate in an upward direction, thus making the problem of pollution more severe. It should be understood that the reasons for the transformation of big cities into "urban heat islands" is attributed to anthropogenic factors. Hence, collective efforts should be made in the task of reducing the urban heat island and for the creation of cooler and healthier cities.

The effect of mesoscale wind on two dimensional air pollution due to an area source is presented using a mathematical model to simulate the dispersion processes of primary pollutants in an urban area with dry deposition and chemical reaction. This model takes into account more realistic forms of large scale wind, mesoscale wind and eddy diffusivity profiles. To clearly visualize the role of mesoscale wind (and hence of urban heat island) in shaping urban

pollution pattern, the whole analysis has also been done in the absence of mesoscale wind and their comparative study shows substantial changes in distribution of pollution. It has been found that the mesoscale wind aggravates the concentrations of air pollutants in the stable and the neutral atmospheric conditions. The results also demonstrated the increase in concentration level up to a considerable height under the mesoscale wind, thus enabling in circulating and moving the pollutants in the vertical direction. It can be concluded that the presence of mesoscale wind enhances the concentration level of the pollutants in urban areas for all vertical and downwind distances under all atmospheric conditions. The analysis reveals that the concentration of the primary pollutants attains peak value at the downwind end of the urban area. In the case of the stable atmospheric condition, the concentration of the primary pollutants is high at the surface region. In the case the neutral atmospheric condition the concentration of the pollutants reaches greater heights. This indicates that the neutral case enhances vertical diffusion of the pollutants. Also, the results obtained from the present work show that in the presence of mesoscale wind, the advection is more on the left side and less on the right side of the centre of heat island. The concentration of the primary pollutants is decreased on the left side and increased on the right side of the centre of heat island in the presence of mesoscale wind as compared to in the absence of mesoscale wind.

Though it is true, that nowadays the air pollution problems are not handled in the way described in the present study, there are various air pollution situations that require the use of complex mesoscale models to adequately describe the processes and dynamics as well as incorporate the knowledge of chemistry and emissions in an adequate manner. Complex modeling studies such as CMAQ (Community Multiscale Air Quality Modeling) have been designed to approach air quality as a whole by including the state of the science capabilities for modeling multiple air quality issues. However, in such complex models, a number of processes going on inside the cities namely; sea breeze circulations, urban heat islands, lee waves etc. to appear as black boxes and one cannot easily understand the effects of individual processes on the air quality. Apart from this, for many policy and scientific applications on air quality modeling, it is desirable not only to know the ambient pollutant concentrations that would result from a certain situation, but also the extent to which those concentrations would change under various perturbations. Thus, the model proposed here helps in understanding one of these processes that is, urban heat island effect, by allowing control over environmental parameters. Hence, it would be easy to determine the steering factor for such a phenomenon and also to test its sensitivity against changes in atmospheric conditions. Thus, the results of the proposed model can be used to increase the level of credibility in complex model predictions and identify variables like wind field, atmospheric stability, etc. which should be investigated more closely in such complex modeling studies.

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